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Expert Systems for the Laboratory: Triple Quadrupole Mass Spectrometry (TQMS) (A Capsule Report on "Expert System" for A/C Interface

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Expert Systems for the Laboratory: Triple Quadrupole Mass Spectrometry (TQMS)

(Capsule Report on "Expert System" for A/C Interface)

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Problem Area. Lawrence Livermore National Laboratory (LLNL), is implementing an expert system for instrument control of a totally computerized triple quadrupole mass spectrometer (TQMS). This system is an ideal candidate for self-adaptive or "knowledge-based" control for several reasons. The spectrometer is a very complex instrument with over 30 computer controlled parameters, and it produces vast amounts of data. Most importantly, the skill required for tuning or optimizing operational conditions is the kind of knowledge that can be represented as procedures and rules (1).

Triple quadrupole mass spectrometers are multi-stage instruments consisting of an ion source, quadrupole mass analyzer, an rf-only quadrupole collision gas chamber, a second quadrupole mass analyzer and an ion detector (2). Figure 1 shows the basic operational modes. It also shows the opportunities for the varied experimental data that can be collected and the increased operational complexity inherent in such systems. The problem is how to optimize for the most significant data, as opposed to merely collecting the most data. In order to do this, one must encode into a knowledge base a tuning procedures for the TQMS which includes heuristics to describe what will eventually become a self-adaptive, feedback control process for real-time optimization of the data acquisition procedure.

Data Structure and Language. The TQMS tuning program is implemented in the knowledge representation language KEE (Knowledge Engineering Environment) developed by IntelliGenetics. This sits on top of the Interlisp-D language running on a Xerox LISP Processor. KEE includes an integrated, object-oriented knowledge representation system and a rule-based reasoning system. The knowledge base includes a set of relateo "objects" or "units". The units describe a concept in terms of its attributes, the actions it can perform, and its relations to other units. The units have a hierarchical relationship (3,4).

Units can pass their attributes to other units in a process called inheritance. Inheritance allows economical information storage because an attribute that is shared by many units is stored in only one. These attributes can either describe a unit, such as the optimum voltage, or delineate the procedures that the unit can perform. One of the procedures that units can perform is to display a graphical representation, or icon of itself, such as the schematic diagram in Figure 2 (3,4).

Search Strategy and Examples. Production rules of the form:

IF <premise> THEN <conclusion>

are used. The control structure involves a "backward chained" search strategy. A conclusion is viewed as an initial hypothesis which is assumed to be true. The initial hypothesis that is stated explicitly in a slot in the unit CALIBRATION is- "that the device is tuned or calibrated". The rule interpreter then tests whether there is evidence for the truth of the hypothesis.

In addition to back-chained rules, the tuning program uses instructions that are interpreted sequentially. Examples of the rule structure and sequential instructions are shown below and are described in more detail elsewhere (3,4).

```
(RULE D)
(IF (DETECTOR OUTPUT IS MAXIMIZED AFTER VARYING LENS1-Q1 VOLTAGE)
    (DETECTOR OUTPUT IS MAXIMIZED AFTER VARYING LENS2-Q1 VOLTAGE)
        •
        •
        •
    (DETECTOR OUTPUT IS MAXIMIZED AFTER VARYING Q3 BIAS-VOLTAGE)
    (THEN (DETECTOR IS COARSE-TUNED)))
```

Sequential instructions have the same syntax as rule preconditions.

```
    (RESET CALIBRATION WORKING-MEMORY)
    (INITIALIZE LENS1-Q1 BIAS VOLTAGE)
    (INITIALIZE LENS2-Q1 BIAS VOLTAGE)
        •
        •
        •
    (ALLOCATE DETECTOR NET-PEAK-WIDTH)
    (CLEAR STATE CALIBRATON-MODE)
    (TEST-HYPOTHESIS CALIBRATION IS SUCCESSFUL)
```

This overall procedure is described in the top-level TQMSTUNE rule shown below:

```
(RULE D2)
(IF (DETECTOR IS COARSE-TUNED)
    (DETECTOR IS FINE-TUNED))
(THEN (CALIBRATION IS SUCCESSFUL)))
```

Strengths and Weaknesses. The primary strengths of using a system like KEE is that it provides a development tool that enables you to encode knowledge very rapidly and to modify and change it very easily. KEE's primary weaknesses are that in the object hierarchy you can only define specific objects, not classes, with instances. The rules structure also cannot invoke itself recursively.

Future. The TQMS tuning procedure can be done much more rapidly via an expert system. A novice can use the system rather than requiring an expert mass spectroscopist. However, the most important aspect is not typical instrument tuning over the entire mass range, but the ability to do on-line real-time optimization of the data selection, acquisition, and interpretation.

An issue that has surfaced repeatedly in mass spectrometry focuses on the number of GC/MS instruments available to be used vs. the number of skilled mass spectrometrists available to operate them. This problem becomes even more critical when dealing with the operation and data interpretation of MS/MS and hyphenated instrument systems such as GC/MS-FTIR. This problem cannot be solved by normal university training programs. Therefore, it is essential to capture the expertise of instrument operators and data interpreters in an expert system. The operation of the complex instrument, the acquisition of the most relevant data, and the ultimate interpretation of that data will be readily available to all analytical laboratories, rather than just the few lucky ones having live "experts".

With the rising public concern for toxic and hazardous waste monitoring and the generation of new organic materials daily, the problems of rapid, reliable complex organic analysis must be approached by the "expert system" method because it is not possible for enough people to become "experts" soon enough.

Acknowledgement

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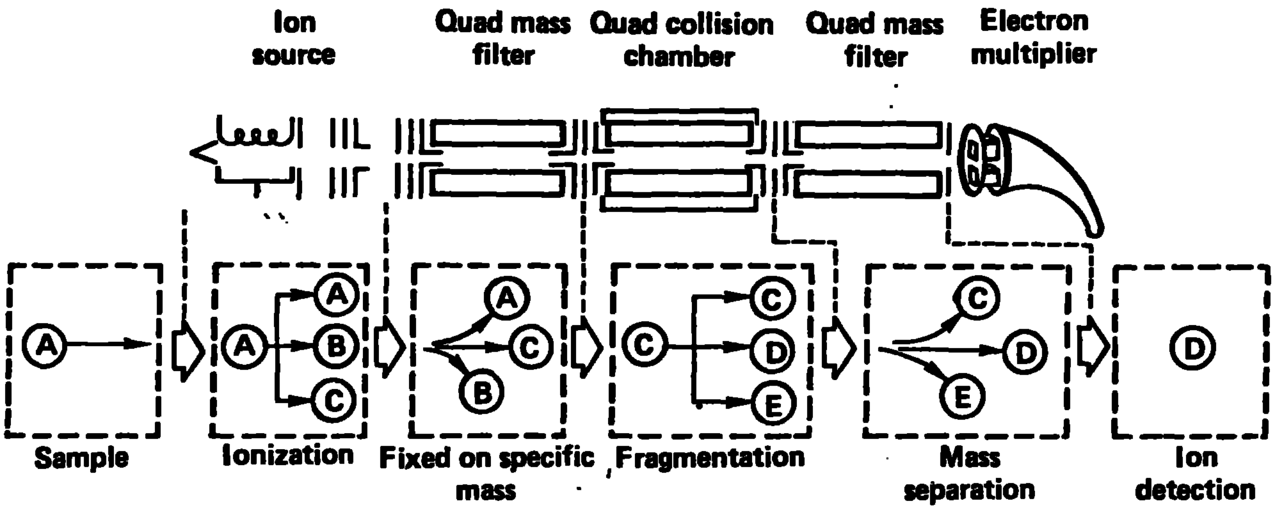

Operation Mode	Quad 1	Quad 2	Quad 3	Results
MS	Separated by mass	All masses passed No gas	All masses passed	Normal mass spectrum
Daughter	Fixed on specific mass	All masses passed Collision gas	Separated by mass	Spectrum of all daughter ions from the selected parent ion
Parent	Separated by mass	All masses passed Collision gas	Fixed on specific mass	Spectrum of parent ions that fragment to give specific daughter ion
Linked	Separated by mass	All masses passed Collision gas	Separated by mass	Fixed mass difference between 2 scanning quads gives specific neutral mass loss
Monitor	Fixed on specific mass	All masses passed Collision gas	Fixed on specific mass	Single or multiple reaction monitoring

Figure 1. Basic operational modes of triple quadrupole mass spectrometer to be controlled by expert system.

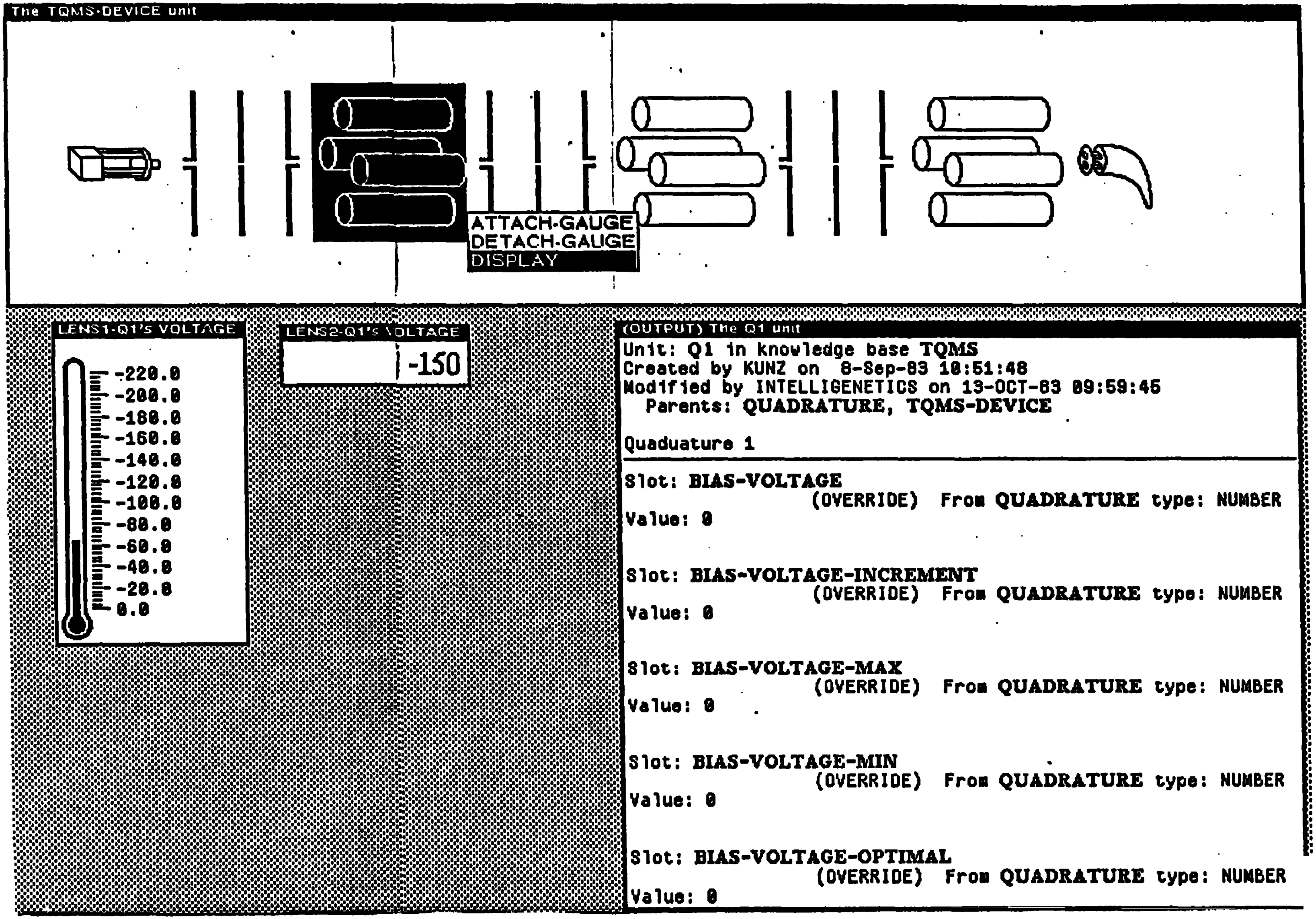

Figure 2. One procedure in the TQMS system allows a unit to display a graphical representation of itself.